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Influence of incommensurability on SDW and CDW amplitudes in underdoped cuprates

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Self-consistent calculations of spin (charge) density wave order (SDW/CDW) parameters have been performed for bilayered cuprates on the basis of a singlet correlated band model. The smooth development of the pseudogap formation temperature is explained from underdoped to overdoped states and the Fourier amplitudes $< s_q >$ (spin) and $< e_q >$ (charge) modulations have been calculated. We have found a maximum of the incommensurability for doping $0.09 \div 0.11$ holes per copper site.

1. Basic relations

We start from the Hamiltonian:

$$H = \sum t_{ij} \Psi_i^{pd,\sigma} \Psi_j^{\sigma,dp} + \sum J_{ij}[2(s_i s_j) - \frac{n_i n_j}{2}] + \\ + \sum g_{ij} \delta_i \delta_j + H_{CDW} \quad (1)$$

where $\Psi_i^{pd,\sigma}$, $\Psi_j^{\sigma,pd}$ are quasiparticle Hubbard-like operators for the copper-oxygen singlet band, J_{ij} is the superexchange constant of the copper spin coupling and g_{ij} is a screened Coulomb repulsion of the doped holes, $1 + \delta_i = \sum_\sigma \Psi_i^{\sigma,\sigma} + 2\Psi_i^{pd,pd}$. The quasiparticle interaction H_{CDW} mediated by the phonon field leads to a CDW transition [1]. In addition to the usual mean field approach we have taken into account that anticommutators of Hubbard-like operators can be affected by the doping index level per one unit cell, spin magnetization and charge modulation (non-Fermi statistics effect (NFS)):

$$P_i^\sigma = \Psi_i^{pd,pd} + \Psi_i^{\sigma,\sigma} = \frac{1+\delta_i}{2} + (-1)^{\frac{1}{2}-\sigma} s_i^z \quad (2)$$

The appearence of SDW and CDW we describe via the Fourier component:

$$s_{q_s}^z = \frac{1}{N} \sum s_i^z \exp(i q_s R_i),$$
$$e_{q_e} = \frac{1}{N} \sum \delta_i \exp(i q_e R_i) \quad (3)$$

where q_s and q_e are the instability wave vectors with respect to SDW and CDW formation. Below we consider both as commensurate wave vectors $q_s = q_e = (\pi, \pi)$ and incommensurate wave vectors $q_s = q_e = (\pi \pm \varepsilon_x, \pi \pm \varepsilon_y)$. In the framework of a linear approximation we can write the equation for the order parameter:

$$\eta_{k+q}^\sigma = [t_{k+q} - \frac{4}{(1+\delta_0)^2} < s_i s_j > t_k] \times \\ < \frac{e_q}{2} - (-1)^{\frac{1}{2}-\sigma} s_q^z > + G_{k+q}^\sigma + G_k^{ph} \quad (4)$$

The CDW order parameters G_{k+q}^σ and G_k^{ph} are determined as in [2]. The thermodynamic values of the Fourier component $< e_q >$ and $< s_q >$ are calculated self-consistently:

$$e_q = \frac{1}{2} \sum_k [< \Psi_{k+q}^{pd,\sigma} \Psi_k^{\sigma,pd} > + < \Psi_{k+q}^{pd,\bar{\sigma}} \Psi_k^{\bar{\sigma},pd} >]$$
$$s_q^z = \frac{1}{2} \sum_k [< \Psi_{k+q}^{pd,\bar{\sigma}} \Psi_k^{\bar{\sigma},pd} > - < \Psi_{k+q}^{pd,\sigma} \Psi_k^{\sigma,pd} >] \quad (5)$$

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